

Bethe Ansatz solution of the small polaron with nondiagonal boundary terms

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Abstract

The small polaron with generic, nondiagonal boundary terms is investigated within the framework of quantum integrability. The eigenvalues of the model are extracted by using the fusion hierarchy of the transfer matrices and the corresponding Bethe Ansatz equations are presented. For particular values of the anisotropy parameter the fusion hierarchy truncates, giving rise to a set of functional relations for the transfer matrix. Exploiting the latter ones, the same set of eigenvalues is rederived, confirming our results. Finally, we comment on the eigenvectors of the model and explicitly compute the state with all sites unoccupied for arbitrary chain lengths.

1 Introduction

The investigation of exactly solvable models over the last many years has been proven very fruitful in extracting physical information regarding phenomena lying in strongly coupled regimes [1]. For integrable models in one spatial dimension, the framework of quantum inverse scattering method (QISM) [2, 3] provides an efficient way of computing the various physical quantities. In the present article we study the small polaron model, which can be also regarded as a graded version of the XXZ quantum spin chain. The R -matrix satisfies the graded Yang-Baxter equation [4, 5, 6]

$$R_{12}(\lambda) R_{13}(\lambda + \mu) R_{23}(\mu) = R_{23}(\mu) R_{13}(\lambda + \mu) R_{12}(\lambda), \quad (1.1)$$

and the resulting bulk Hamiltonian coincides with the bulk Hamiltonian of the XXZ spin chain, after employing a Jordan-Wigner transformation. The effects of supersymmetry become visible when periodicity of the boundary conditions is relaxed, hence more general boundaries are considered, corresponding to open boundaries in the spin chain picture.

Within a graded version of Sklyanin's reflection algebra [7] these boundary conditions can be implemented while keeping the integrability of the model. For purely diagonal boundary fields, i.e. respecting the $U(1)$ symmetry of the bulk, the spectrum of the model can be obtained using algebraic Bethe Ansatz (ABA) methods. For non diagonal boundary conditions, however, this symmetry is broken and a simple reference state does not exist anymore, rendering the ABA framework insufficient. For the respective ungraded model various methods have been successfully employed in the past, such as the fusion hierarchy of the transfer matrices and its truncation [9, 10], the construction of a vacuum state by using gauge transformations [11], generalized TQ equations [12] as well as functional relations derived directly from the Yang-Baxter algebra [13] and by separation of variables [14, 15, 16] amongst others. Nevertheless, in all of these approaches the actual solution of the eigenvalue problem relies on the boundary parameters satisfying certain algebraic relations or is restricted to particular values of the bulk anisotropy parameter.

Motivated by a recent analysis of the free fermion case [17] where the Grassmannian nature of the nondiagonal boundary parameters was proven sufficient to solve the model without imposing any constraints, we studied the small polaron model with nondiagonal boundary conditions, expecting that a similar situation may also hold. As it will become transparent in the next sections, it turns out that this is the case for the interacting fermions as well: supersymmetry lifts the need of imposing constraints on the boundary parameters.

Furthermore, the structure of the eigenvectors is greatly restricted, so that certain eigenstates can be computed exactly for an arbitrary number of chain sites.

The paper is organized as follows: first, we describe the basic facts of the small polaron model and setup our conventions. In Section 3 we study the eigenvalue problem for the transfer matrix (and consequently the Hamiltonian) with non-diagonal boundary conditions based on the fusion hierarchy obtained in [18]. Assuming the existence of a particular limit the spectral problem can be formulated as a functional equation which in turn can be solved by deformation of the corresponding problem in the diagonal case. The transfer matrix eigenvalues are found to depend on two distinct sets of Bethe roots, which satisfy two coupled sets of Bethe Ansatz Equations (BAE). In Section 4 we study the same problem restricted to particular values of the anisotropy parameter, for which truncation identities of the fusion hierarchy were found [18]. The functional relations for the transfer matrix are derived and written into a vanishing determinant representation, which leads to the TQ equation without the need of additional assumptions. The eigenvalues of the transfer matrix coincide exactly with those obtained directly from the fusion hierarchy, thus ensuring the validity of our results. In Section 5 we compute the 'vacuum eigenstate' of the model, i.e. the unique state which reduces to the Fock vacuum in the limit of diagonal boundary fields. Based on this result we propose an expression for the generic structure of the eigenvectors of the model which allows for a complete solution of the spectral problem in principle. We conclude with discussing our results and future directions.

2 The small polaron with open boundary conditions

The small polaron model [19, 20] describes the motion of an additional electron in a polar crystal. The physics of these interactions is captured by the following bulk Hamiltonian

$$H_{\text{bulk}} = \sum_{j=1}^{N-1} -t \left(c_{j+1}^{\dagger} c_j + c_j^{\dagger} c_{j+1} \right) + V \left(n_{j+1} n_j + \bar{n}_{j+1} \bar{n}_j \right), \quad (2.1)$$

where c_k^{\dagger} and c_k denote the creation and annihilation operators of spinless fermions at site k respectively, obeying anticommutation relations $\{c_k^{\dagger}, c_l\} = \delta_{kl}$. We have also introduced the occupation number operators $n_k = c_k^{\dagger} c_k$ and $\bar{n}_k = 1 - n_k$, so that the parameters t and V may be interpreted as hopping amplitude and density-density interaction strength respectively. It is possible to derive the above Hamiltonian through the QISM framework, thus rendering the system integrable [21]. In the Hamiltonian (2.1), periodic boundary conditions are to

be assumed. However, periodicity can be relaxed and one may consider integrable open boundary conditions, by using the framework of quantum integrability for models with open boundaries [7]. The full Hamiltonian of the system contains the additional boundary terms, which in general may be non-diagonal ones

$$H = H_{\text{bulk}} + H_{\text{diag}} + H_{\text{nondiag}}.$$

Since we deal with a fermionic lattice model, the local space of states is \mathbb{Z}_2 -graded [23]. The tensor product is graded according to the rule

$$(A \otimes_s B)^{ac}_{bd} = (-1)^{[p(a)+p(b)]p[c]} A^a_b B^c_d, \quad (2.2)$$

where the parity $p(a)$ is equal to zero (one) for bosonic (fermionic) indices. All matrix operations below, such as the super trace of a matrix, are then to be understood as operations on super matrices. We omit the definitions of these matrix operations and refer the interested reader to the references [22, 23], whose conventions we follow.

The fundamental super transfer matrix of the model is given by the super trace

$$t(u) = \text{str}_0 \left\{ K^+(u) T(u) K^-(u) \hat{T}(u) \right\}, \quad (2.3)$$

where the monodromy matrices are defined as

$$T(u) = R_{N0}(u) \cdots R_{20}(u) R_{10}(u), \quad \hat{T}(u) = R_{01}^{-1}(-u) R_{02}^{-1}(-u) \cdots R_{0N}^{-1}(-u). \quad (2.4)$$

The R -matrix is given by

$$R(u) = \frac{1}{\sin(2\eta)} \begin{pmatrix} \sin(u+2\eta) & 0 & 0 & 0 \\ 0 & \sin(u) & \sin(2\eta) & 0 \\ 0 & \sin(2\eta) & \sin(u) & 0 \\ 0 & 0 & 0 & -\sin(u+2\eta) \end{pmatrix}, \quad (2.5)$$

satisfies the graded Yang-Baxter equation and enjoys several useful properties, such as unitarity

$$R_{12}(u) R_{21}(-u) = \zeta(u), \quad (2.6)$$

crossing symmetry

$$R_{21}^{st_2}(-u-4\eta) R_{21}^{st_1}(u) = \zeta(u+2\eta), \quad (2.7)$$

and periodicity

$$R_{12}(u+\pi) = -\sigma_1^z R_{12}(u) \sigma_1^z = -\sigma_2^z R_{12}(u) \sigma_2^z. \quad (2.8)$$

In the above we have also defined

$$\zeta(u) \equiv g(u)g(-u), \quad \text{and} \quad g(u) \equiv \frac{\sin(u - 2\eta)}{\sin(2\eta)}. \quad (2.9)$$

The K -matrices, which contain the boundary information, satisfy the graded reflection algebra [7, 8] and have the following generic expressions

$$K^-(u) = \omega^- \begin{pmatrix} \sin(u + \psi_-) & \alpha^- \sin(2u) \\ \beta^- \sin(2u) & -\sin(u - \psi_-) \end{pmatrix} \quad (2.10)$$

$$K^+(u) = \omega^+ \begin{pmatrix} \sin(u + 2\eta + \psi_+) & \alpha^+ \sin(2u + 4\eta) \\ \beta^+ \sin(2u + 4\eta) & \sin(u + 2\eta - \psi_+) \end{pmatrix},$$

with normalizations ω^\pm defined by

$$\omega^- \equiv \frac{1}{\sin \psi_-} \quad \text{and} \quad \omega^+ \equiv \frac{1}{2 \cos 2\eta \sin \psi_+}. \quad (2.11)$$

The boundary parameters ψ_\pm are even Grassmann numbers with a non-vanishing complex part, while the parameters α^\pm, β^\pm are odd Grassmann numbers, being subject to the condition $\alpha^\pm \cdot \beta^\pm = 0$. Through the framework of QISM, the super transfer matrix (2.3) gives rise to a commutative family of conserved charges, among them lies the Hamiltonian of the small polaron with open boundaries, which can be derived as

$$\left. \frac{d}{du} t(u) \right|_{u=0} = 2H + \text{const.} \quad (2.12)$$

and coincides with the expressions (2.1), (2), after identifying $t = -\csc 2\eta$ and $V = \cot 2\eta$. The boundary terms read as

$$\begin{aligned} H_{\text{diag}} &= \mathcal{N}_+ \bar{n}_N - \mathcal{N}_- n_N + \frac{1}{2} \cot \psi_- (\bar{n}_1 - n_1) \\ H_{\text{nonddiag}} &= \csc \psi_- (\alpha^- c_1 - \beta^- c_1^\dagger) + \csc \psi_+ (\alpha^+ c_N - \beta^+ c_N^\dagger), \end{aligned} \quad (2.13)$$

where the following shorthands have been also introduced: $\mathcal{N}_\pm \equiv \frac{1}{2} \csc(2\eta) \csc(\psi_\pm) \sin(2\eta \pm \psi_\pm)$.

The super transfer matrix enjoys crossing symmetry

$$t(-u - 2\eta) = \left(\frac{\zeta(u)}{\zeta(-u - 2\eta)} \right)^N t(u), \quad (2.14)$$

and periodicity

$$t(u + \pi) = t(u). \quad (2.15)$$

For future use, we also note that the open transfer matrix is normalized as $t(0) = \mathbb{1}$ and becomes diagonal in the semi-classical limit $\eta \rightarrow 0$

$$t(u)\Big|_{\eta=0} = \frac{(-1)^N}{\sin \psi_+ \sin \psi_-} \left[2 \sin^2 u \cos^2 u (\beta^+ \alpha^- - \alpha^+ \beta^-) \prod_{k=1}^N \sigma_k^z - (\cos^2 u \sin \psi_- \sin \psi_+ + \sin^2 u \cos \psi_- \cos \psi_+) \mathbb{1} \right]. \quad (2.16)$$

Finally, taking the limit $z \equiv e^{iu} \rightarrow \infty$, the asymptotic behavior of the super transfer matrix is obtained, which is needed for later comparison. The leading term contains only odd Grassmann boundary parameters and has the expression

$$t(z) = (-1)^N \frac{\omega^+ \omega^-}{4} z^4 e^{4i\eta} (\beta^+ \alpha^- - \alpha^+ \beta^-) \prod_{j=1}^N (\bar{n}_j - e^{2i\eta} n_j)(n_j + e^{2i\eta} \bar{n}_j) + \mathcal{O}(z^2). \quad (2.17)$$

This particular combination of the odd Grassmann boundary parameters emerges in many different relations, and as will become transparent below it appears uniquely in all eigenvalues of the transfer matrix, thus henceforth it will be denoted as

$$\mathcal{G} \equiv \beta^+ \alpha^- - \alpha^+ \beta^-. \quad (2.18)$$

3 Bethe Ansatz solution from the fusion hierarchy

In order to solve the model under consideration, we exploit the fusion hierarchy of the transfer matrices. Having a transfer matrix at hand, one may construct a family of commuting transfer matrices derived from auxiliary spaces of higher dimension, through a suitable fusion procedure [25, 26]. The super quantum determinant of the small polaron is given by

$$\Delta(u) = \left(\frac{\zeta(u+2\eta)}{\zeta(u)} \right)^N g(-2u-6\eta)g(2u+2\eta) \det K^+(u) \det K^-(u+2\eta). \quad (3.1)$$

Note that this expression coincides with the quantum determinant of the model with diagonal boundaries as a consequence of the constraint $\alpha^\pm \cdot \beta^\pm = 0$ for the off-diagonal elements of the boundary matrices. It is useful to introduce the rescaled quantities

$$\tilde{\Delta}(u) \equiv \frac{\Delta(u)}{\zeta(2u+4\eta)}, \quad \text{and} \quad \tilde{t}^{(n)}(u) \equiv - \left(\prod_{i=1}^{n-1} \xi_i^{-1}(u) \right) t^{(n)}(u), \quad (3.2)$$

with $\tilde{t}^{(0)} \equiv -t^{(0)} \equiv \mathbb{1}$ and $\tilde{t}^{(1)} \equiv t^{(1)}(u) \equiv -t(u)$ and

$$\xi_n(u) \equiv \prod_{k=1}^n \zeta(2u + [n+k] \cdot 2\eta). \quad (3.3)$$

In terms of these rescaled quantities, the fusion hierarchy reads as [18]

$$\tilde{t}^{(n)}(u) \cdot \tilde{t}^{(1)}(u + n \cdot 2\eta) = \tilde{t}^{(n+1)}(u) - \tilde{\Delta}(u + [n - 1] \cdot 2\eta) \cdot \tilde{t}^{(n-1)}(u). \quad (3.4)$$

Since the fused transfer matrices commute with each other, the fusion hierarchy can be also read as a set of relations between their eigenvalues, which after shifting $u \rightarrow u - n \cdot 2\eta$ gives

$$\tilde{\Lambda}(u) = \frac{\tilde{\Lambda}^{(n+1)}(u - n \cdot 2\eta)}{\tilde{\Lambda}^{(n)}(u - n \cdot 2\eta)} - \tilde{\Delta}(u - 2\eta) \frac{\tilde{\Lambda}^{(n-1)}(u - n \cdot 2\eta)}{\tilde{\Lambda}^{(n)}(u - n \cdot 2\eta)}. \quad (3.5)$$

Assuming that the limit $\tilde{Q}(u) = \lim_{n \rightarrow \infty} \tilde{\Lambda}^{(n)}(u - n \cdot 2\eta)$ exists then [27], one obtains the formulation of the spectral problem as a TQ-equation from the fusion hierarchy

$$\tilde{\Lambda}(u) = H_\alpha(u) \frac{\tilde{Q}(u - 2\eta)}{\tilde{Q}(u)} - H_\delta(u) \frac{\tilde{Q}(u + 2\eta)}{\tilde{Q}(u)}, \quad (3.6)$$

the sole requirement being that the H -functions should factorize the quantum determinant as $H_\delta(u - 2\eta)H_\alpha(u) = \zeta^{-1}(2u)\Delta(u - 2\eta)$.

Since the diagonal case should be contained within the construction as a special limit, we propose the following deformations of the H -functions

$$H_{\alpha,\delta}(u) = h_{\alpha,\delta}(u)(1 + \mathcal{G} f_{\alpha,\delta}(u)), \quad (3.7)$$

where $h_{\alpha,\delta}(u)$ are the h -functions of the diagonal case, which essentially factorize the quantum determinant

$$\begin{aligned} h_\alpha(u) &= \omega^+ \omega^- \frac{\sin(2u + 4\eta)}{\sin(2u + 2\eta)} \sin(u + \psi_+) \sin(u + \psi_-) \left(\frac{-\sin(u + 2\eta)}{\sin(u - 2\eta)} \right)^N \\ h_\delta(u) &= \omega^+ \omega^- \frac{\sin 2u}{\sin(2u + 2\eta)} \sin(u + 2\eta - \psi_+) \sin(\psi_- - u - 2\eta) \left(\frac{-\sin^2 u}{\sin(u + 2\eta) \sin(u - 2\eta)} \right)^N, \end{aligned} \quad (3.8)$$

and $f_{\alpha,\delta}(u)$ are generic functions to be determined. There exist two constraints on the expressions of these unknown functions. First, their contribution in the factorization of the quantum determinant should vanish, yielding

$$f_\delta(u - 2\eta) = -f_\alpha(u). \quad (3.9)$$

Furthermore, assuming that the \tilde{Q} -functions have crossing symmetry, the H -functions are related through $\zeta^N(u) H_\alpha(u) = -\zeta^N(-u - 2\eta) H_\delta(-u - 2\eta)$. This relation holds automatically for the h -functions of the diagonal case, whereas it also provides a second constraint on $f_{\alpha,\delta}(u)$:

$$f_\delta(-u - 2\eta) = f_\alpha(u). \quad (3.10)$$

A set of solutions to these functional relations is given by

$$\begin{aligned} f_\delta(u) &= \mathcal{W} \sin(2u + 4\eta) \\ f_\alpha(u) &= -\mathcal{W} \sin(2u), \end{aligned} \quad (3.11)$$

with the coefficient \mathcal{W} to be determined from the asymptotic behavior (2.17) of the transfer matrix eigenvalues. It should be stressed out that the above choice is not unique, but it was found to be the only one consistent with the various limits and with the constraints arising from the functional relations, as they will be described in the following section.

For the nondiagonal case that we investigate, a similar deformation should be considered for the \tilde{Q} -functions as well, since they are assumed to originate from the higher spin eigenvalues through a limiting procedure. The most general ansatz extending the Q -functions of the diagonal case, $Q(u)$, and containing the special combination of Grassmann numbers, \mathcal{G} , reads as

$$\tilde{Q}(u) = Q(u) + \mathcal{G} b(u), \quad Q = \prod_{\ell=1}^M \sin(u - v_\ell^{(0)}) \sin(u + v_\ell^{(0)} + 2\eta), \quad (3.12)$$

with $b(u)$ being a function to be determined. Substituting the deformations (3.7) and (3.12) into the TQ equation, the latter one becomes

$$\begin{aligned} \tilde{\Lambda}(u) = \tilde{\Lambda}^{\text{diag}}(u) &\left(1 - \mathcal{G} \frac{b(u)}{Q(u)}\right) + \mathcal{G} \left[h_\alpha(u) \left(\frac{b(u - 2\eta)}{Q(u)} + f_\alpha(u) \frac{Q(u - 2\eta)}{Q(u)} \right) \right. \\ &\left. - h_\delta(u) \left(\frac{b(u + 2\eta)}{Q(u)} + f_\delta(u) \frac{Q(u + 2\eta)}{Q(u)} \right) \right], \end{aligned} \quad (3.13)$$

with the eigenvalues of the diagonal case being given by the relation

$$\tilde{\Lambda}^{\text{diag}}(u) = h_\alpha(u) \frac{Q(u - 2\eta)}{Q(u)} - h_\delta(u) \frac{Q(u + 2\eta)}{Q(u)}. \quad (3.14)$$

Note that only the Q -functions of the diagonal case appear in the denominator of $\tilde{\Lambda}(u)$. Therefore, their zeros $v_\ell^{(0)}$ are determined by requiring analyticity of the eigenvalues of the transfer matrix, in particular of their diagonal part $\tilde{\Lambda}^{\text{diag}}(u)$. This yields the BAE

$$\frac{h_\alpha(v_\ell^{(0)})}{h_\delta(v_\ell^{(0)})} = \frac{Q(v_\ell^{(0)} + 2\eta)}{Q(v_\ell^{(0)} - 2\eta)}, \quad (3.15)$$

or upon substitution

$$\begin{aligned} \left(\frac{\sin(v_\ell^{(0)} + 2\eta)}{\sin v_\ell^{(0)}} \right)^{2N} &\frac{\sin(v_\ell^{(0)} + \psi_-) \sin(v_\ell^{(0)} + \psi_+)}{\sin(v_\ell^{(0)} + 2\eta - \psi_+) \sin(v_\ell^{(0)} + 2\eta - \psi_-)} = \\ &= \prod_{j \neq \ell}^M \frac{\sin(v_\ell^{(0)} - v_j^{(0)} + 2\eta) \sin(v_\ell^{(0)} + v_j^{(0)} + 4\eta)}{\sin(v_\ell^{(0)} - v_j^{(0)} - 2\eta) \sin(v_\ell^{(0)} + v_j^{(0)})}. \end{aligned} \quad (3.16)$$

In the case of nondiagonal boundaries, additional requirements are needed to determine the function $b(u)$ in (3.12). Again the choice of this function has to guarantee the analyticity of the additional terms appearing in the functional equation (3.13) for the eigenvalues. In addition, $b(u)$ should enjoy crossing symmetry. In this spirit, we propose that the nondiagonal correction to the \tilde{Q} -functions is given by

$$b(u) = \prod_{\ell=1}^{M'} \sin(u - v_\ell^{(1)}) \sin(u + v_\ell^{(1)} + 2\eta), \quad (3.17)$$

with $\{v_\ell^{(1)}\} \neq \{v_\ell^{(0)}\}$ in general. Matching of the asymptotic behavior dictates that the upper limits of the products in eqs. (3.12) and (3.17) should be equal, $M' = M$. Furthermore, the asymptotics (2.17) provide the explicit expression for the coefficient \mathcal{W} as

$$\mathcal{W} = \frac{1}{\sin[\psi_+ + \psi_- + (N - 2M - 1)2\eta]}. \quad (3.18)$$

Apart from the asymptotics, one should also consider additional limits of the TQ equation in order to check the consistency of the procedure. The limit $u \rightarrow 0$ gives $\tilde{\Lambda}(0) = 1$, which stems from the normalization of the transfer matrix. Setting $u = 0$ in the TQ equation, after a quick inspection one is lead to the following constraint for $b(u)$

$$b(-2\eta) = b(0), \quad (3.19)$$

which is a special case of a crossing symmetry requirement and automatically satisfied by the choice (3.17). Finally, it is interesting to consider the semi-classical limit $\eta \rightarrow 0$. In this limit the $b(u)$ functions drop out from the TQ equation and the eigenvalues become

$$\tilde{\Lambda}(u) \Big|_{\eta \rightarrow 0} = (h_\alpha(u) - h_\delta(u)) + \mathcal{G} f_\alpha(u) (h_\alpha(u) + h_\delta(u)), \quad (3.20)$$

finding perfect agreement with the semi-classical limit obtained from the transfer matrix (2.16), after recalling the definitions (3.8), the solutions (3.11) and the expression (3.18) of the coefficient \mathcal{W} for $\eta \rightarrow 0$.

The parameters $v_\ell^{(1)}$ in (3.17) are determined by requiring analyticity of the eigenvalues of the transfer matrix for the nondiagonal case. The purely complex part of the TQ equation (3.13) yields the already derived BAE (3.16), while the one containing Grassmann numbers provides a second set of relations, involving both sets of roots $v^{(0)}$, $v^{(1)}$, which reads as

$$\frac{h_\alpha(v_\ell^{(0)})}{h_\delta(v_\ell^{(0)})} = \frac{\tilde{\Lambda}^{\text{diag}}(v_\ell^{(0)}) b(v_\ell^{(0)})}{h_\delta(v_\ell^{(0)}) \left(b(v_\ell^{(0)} - 2\eta) + f_\alpha(v_\ell^{(0)}) Q(v_\ell^{(0)} - 2\eta) \right)} + \frac{b(v_\ell^{(0)} + 2\eta) + f_\delta(v_\ell^{(0)}) Q(v_\ell^{(0)} + 2\eta)}{b(v_\ell^{(0)} - 2\eta) + f_\alpha(v_\ell^{(0)}) Q(v_\ell^{(0)} - 2\eta)}. \quad (3.21)$$

Note that the roots $v^{(0)}$ and $v^{(1)}$ also enter this set of equations through the functions $Q(u)$ and $b(u)$.

In summary, we have two sets of algebraic equations fixing the parameters appearing in the ansatz for $\tilde{Q}(u)$. These equations are of nested Bethe Ansatz type, similar to those appearing in integrable models based on higher rank symmetries.

In order to further test our proposed expressions for the eigenvalues as computed from the TQ equation, we have analytically diagonalized the transfer matrix for a small number of chain lengths. The comparison of the exact eigenvalues with the ones obtained from (3.13) exhibits perfect agreement.

4 Truncation of the fusion hierarchy and functional relations

The findings of the previous section are based on the assumption that the limit $\tilde{Q}(u) = \lim_{n \rightarrow \infty} \tilde{\Lambda}^{(n)}(u - n \cdot 2\eta)$ exists. In order to enforce the validity of our results, we follow here a different path. For particular values of the quasi-classical parameter, $\eta_n = \frac{\pi/2}{n+1}$, the fusion hierarchy truncates and the derived functional relations can be used to derive the TQ equation. The truncation identities have been worked out in [18], where it was found that¹

$$\tilde{t}^{(n)}(u, \eta_{n-1}) = \phi_{n-1}^{\text{id}}(u) \cdot \mathbb{I} - \phi_{n-1}^\tau(u) \cdot \tilde{t}^{(n-2)}(u + 2\eta_{n-1}, \eta_{n-1}), \quad (4.1)$$

where the functions $\phi_n^{\text{id}}(u), \phi_n^\tau(u)$ are given by the following expressions

$$\begin{aligned} \phi_n^{\text{id}}(u) &= \mathcal{M}_n^{2N}(u) \mu_n^+(u) \mu_n^-(u) [\nu_n^+(-u) \nu_n^-(u) + \nu_n^+(u) \nu_n^-(-u)] \\ \phi_n^\tau(u) &= \zeta^{2N}(u) \mu_n^+(u) \mu_n^-(u), \end{aligned} \quad (4.2)$$

with

$$\begin{aligned} \mathcal{M}_n(u) &\equiv \left(\frac{1/2}{\sin 2\eta_n} \right)^n \frac{\sin([n+1]u)}{\sin 2\eta_n} \\ \mu_n^\pm(u) &\equiv \pm \delta\{K^\pm(\mp u - 2\eta_n, \eta_n)\} \frac{\sin(2\eta_n)}{\sin(2u - 2 \cdot 2\eta_n)} \prod_{k=2}^{2n} \frac{\sin(2u + k \cdot 2\eta_n)}{\sin(2\eta_n)} \\ \nu_n^\pm(u) &\equiv \mp \frac{\omega_n^\pm}{\mu_n^\pm(u)} \left(\frac{\omega_n^\pm}{2} \right)^n \sin([n+1][u \mp \psi_\pm]) \prod_{i=1}^n \prod_{j=1}^i \frac{\sin(2u + [i+j] \cdot 2\eta_n)}{\sin(2\eta_n)}. \end{aligned} \quad (4.3)$$

¹Note that in the present section we use a slightly different normalization for the transfer matrix. In contrast to (2.4), now $\hat{T}(u) = R_{01}(u)R_{02}(u) \cdots R_{0N}(u)$.

Combining the fusion hierarchy with the truncation identity for a particular value n , yields an $(n + 1)$ -order functional equation for the transfer matrix of the model. Unfortunately, it does not seem plausible to write the functional relations in a closed form. Starting from low values of n , one observes that at each level new terms emerge and their number is given by the Fibonacci numbers. In particular, at a given value n , there are

$$F(n + 1) + F(n - 1) + 1, \quad n = 2, 3, \dots$$

terms in total. Nevertheless, after carefully examining the structure of the functional relations, it is seen that the following simple schematic structure appears

$$\begin{aligned} & \tilde{t}(u) \tilde{t}(u + 2\eta) \cdots \tilde{t}(u + (2n - 2)\eta) + \mathcal{U}_1 + \tilde{\phi}_{n-1}^\tau(u) \cdot \mathcal{U}_0 \\ &= \tilde{\phi}_{n-1}^{id}(u) + \prod_{k=0}^{\frac{n}{2}-1} \tilde{\Delta}(u + 4k\eta) + \tilde{\phi}_{n-1}^\tau(u) \prod_{k=1}^{\frac{n}{2}-1} \tilde{\Delta}(u + (4k - 2)\eta). \end{aligned} \quad (4.4)$$

First, we should note that the last two terms in the RHS are present only for even values of n . Next, the symbol \mathcal{U} stands for the following sequence:

$$\begin{aligned} \mathcal{U}_1 &:= \sum_{q_0=0}^{n-2} \tilde{\Delta}(u + 2q_0\eta) \mathcal{T}_{q_0}(u) \\ &+ \sum_{q_1=0}^{n-4} \tilde{\Delta}(u + (2q_1 + 4)\eta) \sum_{q_0=0}^{q_1} \tilde{\Delta}(u + 2q_0\eta) \mathcal{T}_{q_0q_1}(u) \\ &+ \sum_{q_2=0}^{n-6} \tilde{\Delta}(u + (2q_2 + 8)\eta) \sum_{q_1=0}^{q_2} \tilde{\Delta}(u + (2q_1 + 4)\eta) \sum_{q_0=0}^{q_1} \tilde{\Delta}(u + 2q_0\eta) \mathcal{T}_{q_0q_1q_2}(u) \\ &+ \cdots, \end{aligned} \quad (4.5)$$

with

$$\mathcal{T}_{q_0q_1\cdots q_\ell}(u) \equiv \prod_{\substack{m=0 \\ m \notin \{Q\}}}^{n-1} \tilde{t}(u + 2m\eta), \quad Q = \{q_i + 2i, q_i + 2i + 1\}, \quad i = 1, 2, \dots, \ell.$$

A similar structure holds for \mathcal{U}_0 as well, although some lower/upper limits of the sums and the product are different. Nevertheless, the structure above is reminiscent of a path-ordered exponential, and appears as some deformed discrete version of the latter one. It would be interesting to see if this observation possesses some physical meaning, i.e., if the corresponding operator in the path-ordered exponential plays some physical role here.

Despite the fact that the functional relations cannot be written in a closed form, they can be cast into a vanishing determinant representation, which afterwards provides the TQ equations. The restriction $m \notin Q$ in (4.5) reflects exactly this property.

4.1 The determinant representation

The vanishing determinant representation has the same structure with the corresponding one of the XXZ model [10]. In particular, the functional relations (4.4) take the following form:

$$\det \begin{pmatrix} \tilde{\Lambda}_0 & -\tilde{h}_{-1} & 0 & 0 & \cdots & 0 & 0 & -h_0 \\ -h_1 & \tilde{\Lambda}_1 & -\tilde{h}_0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -h_2 & \tilde{\Lambda}_2 & -\tilde{h}_1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -h_{n-1} & \tilde{\Lambda}_{n-1} & -\tilde{h}_{n-2} \\ -\tilde{h}_{n-1} & 0 & 0 & 0 & \cdots & 0 & -h_n & \tilde{\Lambda}_n \end{pmatrix} = 0, \quad (4.6)$$

where $\tilde{\Lambda}_k \equiv \tilde{\Lambda}(u + 2k\eta)$ is an eigenvalue of $\tilde{t}(u + 2k\eta)$, $h_k = h(u + 2k\eta)$ and $\tilde{h}_k = \tilde{h}(u + 2k\eta)$. The functions h_k, \tilde{h}_k are determined by demanding relations (4.4) and (4.6) to be identical. One concludes then that

$$\begin{aligned} h(u + 2\eta) \tilde{h}(u - 2\eta) &= -\tilde{\Delta}(u), \\ h(u) \tilde{h}(u + 2(n-1)\eta) &= -\tilde{\phi}_n^\tau(u), \end{aligned} \quad (4.7)$$

$$\prod_{k=0}^n h(u + 2k\eta) + \prod_{k=-1}^{n-1} \tilde{h}(u + 2k\eta) = \tilde{\phi}_n^{id}(u).$$

Inspired by the structure of the h -function in the XXZ case [10], as well as the functions found in [18], we consider the following expressions

$$\tilde{h}(u) = h(-u - 4\eta), \quad h(u) = \left(\frac{\sin(u + 2\eta)}{\sin 2\eta} \right)^{2N} \frac{\sin(2u + 4\eta)}{\sin(2u + 2\eta)} g_-(u) g_+(u), \quad (4.8)$$

where the functions $g_\pm(u)$ contain the boundary information. Substituting the above expressions into (4.7), the following condition arises regarding the functions $g_\pm(u)$:

$$g_-(u + 2\eta) g_-(-u - 2\eta) g_+(u + 2\eta) g_+(-u - 2\eta) = \det K^+(u) \det K^-(u + 2\eta). \quad (4.9)$$

Assuming that the functions factorize the determinants of the reflection matrices as

$$\begin{aligned} g_-(u + 2\eta) g_-(-u - 2\eta) &= \det K^-(u + 2\eta) \\ g_+(u + 2\eta) g_+(-u - 2\eta) &= -\det K^+(u), \end{aligned} \quad (4.10)$$

and recalling the explicit expressions for the determinants of the boundary matrices, the relations above are then equivalent to

$$\begin{aligned} g_-(u) g_-(-u) &= \det K^-(u) = -(\omega^-)^2 \sin(u + \psi_-) \sin(u - \psi_-) \\ g_+(u) g_+(-u) &= \det K^+(u) = -(\omega^+)^2 \sin(u + \psi_+) \sin(u - \psi_+), \end{aligned} \quad (4.11)$$

pinpointing to the natural solutions

$$g_-(u) = \omega^- \sin(u + \psi_-), \quad g_+(u) = \omega^+ \sin(u + \psi_+). \quad (4.12)$$

Using the expressions (4.12) then, all three relations in (4.7) are automatically satisfied. It should be stressed out that the construction so far does not involve the boundary odd Grassmann numbers at all. In fact, the structure we have found here is identical with the corresponding structure of the purely diagonal XXZ case [10], since the odd Grassmann parameters drop out from the determinants due to their nature.

The vanishing determinant guarantees the existence of a null vector, (Q_0, Q_1, \dots, Q_n) , so that the following relations hold

$$\begin{aligned} \tilde{\Lambda}_0 Q_0 - \tilde{h}_{-1} Q_1 - h_0 Q_n &= 0, \\ -h_k Q_{k-1} + \tilde{\Lambda}_k Q_k - \tilde{h}_{k-1} Q_{k+1} &= 0, \quad k = 1, \dots, n-1, \\ -\tilde{h}_{n-1} Q_0 - h_n Q_{n-1} + \tilde{\Lambda}_n Q_n &= 0. \end{aligned} \quad (4.13)$$

For the present choice of the quasi-classical parameter, i.e. $\eta = \eta_n = \frac{\pi/2}{n+1}$, these equations can be recast as TQ equations for a periodic function $Q(u)$ by identifying $Q_k = Q(u + 2\eta k)$:

$$\tilde{\Lambda}(u) = h(u) \frac{Q(u - 2\eta)}{Q(u)} + h(-u - 2\eta) \frac{Q(u + 2\eta)}{Q(u)}. \quad (4.14)$$

Note that the h -functions appearing in the relation above essentially factorize the quantum determinant as $h(u)h(-u) = \zeta^{-1}(2u)\Delta(u - 2\eta)$. The derived TQ equation is actually the same with the one obtained directly from the fusion hierarchy, since $h(u)$ may be identified with $h_\alpha(u)$ defined in Eq. (3.8). One may proceed then with the deformation of the h -function, as well as that of the Q -functions to incorporate nondiagonal contributions. We have also checked explicitly that the deformed h -functions (3.11), (3.18) satisfy the two additional constraints arising during the truncation of the hierarchy, that is Eqs. (4.7). Hence the two approaches converge to give the same results.

5 The eigenstates of the model

In the previous sections we have obtained the eigenvalues of the transfer matrix from the the fusion hierarchy and the resulting TQ equation. Similar as in the case of diagonal boundary matrices the eigenvalues can be associated to sectors labelled by the integer M of

parameters appearing in the solution. This is remarkable since the related $U(1)$ symmetry is broken when the nondiagonal boundary conditions are applied.

As is common to functional Bethe Ansatz approaches our solution of the spectral problem thus far does not provide information regarding the eigenstates of the model. However, exploiting the existence of the odd Grassmann numbers and their nilpotency, it is possible to exactly compute the $M = 0$ state of the model for an arbitrary number N of chain sites, solely by using the derived expressions of the eigenvalues. To this end we choose k -particle states, $k = 0, \dots, N$,

$$|i_1 i_2 \dots i_k\rangle \equiv c_{i_1}^\dagger c_{i_2}^\dagger \dots c_{i_k}^\dagger |\Omega\rangle, \quad 1 \leq i_1 < i_2 < \dots < i_k \leq N \quad (5.1)$$

as basis of the Hilbert space of the system, $|\Omega\rangle$ is the Fock vacuum of the system (and the $M = 0$ eigenvector of the diagonal problem).

The key observation used for the construction of the unique $M = 0$ eigenvector of the model with nondiagonal boundary conditions is that for generic chain length N , only the Fock vacuum and basis states containing one or two particles contribute with a non-vanishing amplitude, all other sectors decouple. This allows to express the $M = 0$ eigenvector of the nondiagonal model as

$$|\Psi\rangle_{M=0} = |\Omega\rangle + \beta^+ \sum_{i=1}^N b_i^+ |i\rangle + \beta^- \sum_{i=1}^N b_i^- |i\rangle + \beta^+ \beta^- \sum_{i < j}^N B_{ij} |ij\rangle. \quad (5.2)$$

The eigenvalue problem for the complete Hamiltonian reads as

$$H|\Psi\rangle = (\lambda_{\text{diag}} + \mathcal{G} \lambda_{\text{nondiag}}) |\Psi\rangle. \quad (5.3)$$

Splitting the terms with respect to the order of β^\pm we obtain

$$\begin{aligned} \mathcal{O}(\beta) : \quad & (H_{\text{bulk}} + H_{\text{diag}}) \beta^\kappa \sum_i b_i^\kappa |i\rangle + H_{\text{nondiag}} |\Omega\rangle = \lambda_{\text{diag}} \beta^\kappa \sum_i b_i^\kappa |i\rangle \\ \mathcal{O}(\beta^2) : \quad & (H_{\text{bulk}} + H_{\text{diag}}) \beta^+ \beta^- \sum_{i < j} B_{ij} |ij\rangle + H_{\text{nondiag}} \beta^\kappa \sum_i b_i^\kappa |i\rangle = \\ & = \mathcal{G} \lambda_{\text{nondiag}} |\Omega\rangle + \lambda_{\text{diag}} \beta^+ \beta^- \sum_{i < j} B_{ij} |ij\rangle. \end{aligned} \quad (5.4)$$

Regarding the terms linear in β^\pm first, after the relevant computations and splitting the resulting relations with respect to the appropriate excited states, one ends up with the following six relations that determine the coefficients b_i^\pm

$$\beta^+ |1\rangle : \quad -t b_2^+ + b_1^+ [V(N-2) - \frac{1}{2} \cot \psi_- + \mathcal{N}_+ - \lambda_{\text{diag}}] = 0$$

$$\begin{aligned}
\beta^+|N\rangle : \quad & -t b_{N-1}^+ - \csc \psi_+ + b_N^+ [V(N-2) + \tfrac{1}{2} \cot \psi_- - \mathcal{N}_- - \lambda_{\text{diag}}] = 0 \\
\beta^-|1\rangle : \quad & -t b_2^- - \csc \psi_- + b_1^- [V(N-2) - \tfrac{1}{2} \cot \psi_- + \mathcal{N}_+ - \lambda_{\text{diag}}] = 0 \\
\beta^-|N\rangle : \quad & -t b_{N-1}^- + b_N^- [V(N-2) + \tfrac{1}{2} \cot \psi_- - \mathcal{N}_- - \lambda_{\text{diag}}] = 0 \\
\beta^\pm|\ell\rangle : \quad & -t (b_{\ell-1}^\pm + b_{\ell+1}^\pm) + b_\ell^\pm [V(N-3) + \tfrac{1}{2} \cot \psi_- + \mathcal{N}_+ - \lambda_{\text{diag}}] = 0, \quad (5.5)
\end{aligned}$$

where the recursion relations are valid for $2 \leq \ell \leq N-1$ and can be solved analytically, giving

$$b_\ell^\pm = \frac{1}{2^\ell} \left[\left(\frac{\mathcal{C}_0 - \sqrt{\mathcal{C}_0^2 - 4t^2}}{t} \right)^\ell \mathcal{C}_1^\pm + \left(\frac{\mathcal{C}_0 + \sqrt{\mathcal{C}_0^2 - 4t^2}}{t} \right)^\ell \mathcal{C}_2^\pm \right], \quad (5.6)$$

with $\mathcal{C}_0 \equiv V(N-3) + \tfrac{1}{2} \cot \psi_- + \mathcal{N}_+ - \lambda_{\text{diag}}$ and $\mathcal{C}_{1,2}^\pm$ constants to be determined. Proceeding to the quadratic terms, the ones proportional to $\beta^+ \alpha^-$ and $\beta^- \alpha^+$ first give the constraints

$$\csc(\psi_-) b_1^+ = \lambda_{\text{nondiag}} = \csc(\psi_+) b_N^-. \quad (5.7)$$

These two constraints, combined with the set of relations (5.5) are sufficient to completely determine the constants $\mathcal{C}_{1,2}^\pm$ and therefore all coefficients b_ℓ^\pm . We conclude that the coefficients b_ℓ^\pm are given by

$$\begin{aligned}
b_\ell^+ &= -\frac{\sin(\psi_- + (\ell-1)2\eta)}{\sin((N-1)2\eta + \psi_- + \psi_+)} \\
b_\ell^- &= -\frac{\sin(\psi_+ + (N-\ell)2\eta)}{\sin((N-1)2\eta + \psi_- + \psi_+)}. \quad (5.8)
\end{aligned}$$

Concerning the rest of the quadratic terms, after some algebra and splitting the terms with respect to various states, we conclude that the coefficients $B_{k\ell}$ satisfy the following relations

$$\begin{aligned}
(\Xi_3^+ + \mathcal{N}_-) B_{1N} + t(B_{1N-1} + B_{2N}) + b_N^+ \csc \psi_- + b_1^- \csc \psi_+ &= 0 \\
(\Xi_2^+ - \mathcal{N}_+) B_{12} + t B_{13} + b_2^+ \csc \psi_- &= 0 \\
(\Xi_2^- + \mathcal{N}_-) B_{N-1N} + t B_{N-2N} + b_{N-1}^- \csc \psi_+ &= 0 \\
(\Xi_4^- + \mathcal{N}_-) B_{\ell N} + t(B_{\ell-1N} + B_{\ell+1N} + B_{\ell N-1}) + b_\ell^- \csc \psi_+ &= 0, \quad 1 < \ell < N-1 \\
(\Xi_4^+ - \mathcal{N}_+) B_{1\ell} + t(B_{1\ell-1} + B_{1\ell+1} + B_{2\ell}) + b_\ell^+ \csc \psi_- &= 0, \quad 2 < \ell < N \\
(\Xi_3^- - \mathcal{N}_+) B_{\ell\ell+1} + t(B_{\ell-1\ell+1} + B_{\ell\ell+2}) &= 0, \quad 1 < \ell < N-1 \\
(\Xi_5^- - \mathcal{N}_+) B_{k\ell} + t(B_{k-1\ell} + B_{k+1\ell} + B_{k\ell-1} + B_{k\ell+1}) &= 0, \quad 1 < k < N-2, \quad \ell > k+1
\end{aligned}$$

where for the sake of readability we have defined

$$\Xi_q^\pm \equiv \lambda_{\text{diag}} \pm \tfrac{1}{2} \cot \psi_- - V(N-q). \quad (5.9)$$

In principle, having acquired the exact expressions for b_ℓ^\pm , the above set of relations provides the expressions of $B_{k\ell}$ as well. Since it is hard to solve these relations analytically, one may

resort to a numerical analysis for a given number of chain sites. However, solving these equations for small numbers of chain length, we were able to observe the emerging pattern which governs the coefficients $B_{k\ell}$. In short, we have found that they are eventually given by the very simple expressions

$$B_{k\ell} = \frac{\sin((N-1)2\eta + \psi_- + \psi_+)}{\sin((N-2)2\eta + \psi_- + \psi_+)} (b_{k+1}^+ b_\ell^- + b_k^- b_{\ell-1}^+). \quad (5.10)$$

We have explicitly confirmed that the expressions (5.10) satisfy all the generic constraints and relations derived above. In conclusion, the $M = 0$ eigenvector of the model is completely determined for an arbitrary number of chain sites.

The decoupling of higher/lower sectors, due to the nilpotency of the Grassmannian parameters, further constraints the expressions of the eigenvectors which correspond to excited states. For generic values of M then, we propose that the corresponding eigenvector will be given by the following schematic expression

$$\begin{aligned} |\Psi\rangle_M &= (c_1 + c_2 \alpha^+ \beta^- + c_3 \beta^+ \alpha^-) |M\rangle + c_4 \beta^+ |M+1\rangle + c_5 \beta^- |M+1\rangle \\ &+ c_6 \beta^+ \beta^- |M+2\rangle + c_7 \alpha^+ |M-1\rangle + c_8 \alpha^- |M-1\rangle + c_9 \alpha^+ \alpha^- |M-2\rangle, \end{aligned} \quad (5.11)$$

where with $|M\rangle$ we denote the states with M particles present, or equivalently the states with M spins down in the spin picture, i.e. M excitations from the ground state. The number of states with the same M is given by the binomial coefficient

$$\binom{N}{M} = \frac{N!}{M!(N-M)!}, \quad (5.12)$$

so that the states $|M\rangle$ in (5.11) are to be understood as collections of states spanning the degeneracy space for a particular M . In the same spirit, the coefficients $c_i \in \mathbb{C}$ appearing also in (5.11) are to be interpreted as sets of coefficients of the degenerate states.

6 Discussion

In the present work, we have solved the small polaron model with nondiagonal boundary conditions. The eigenvalues of the transfer matrix have been extracted first by direct use of the fusion hierarchy and then by considering the functional relations for particular values of the anisotropy parameter. Both approaches yield the same set of eigenvalues, confirming our proposed deformations needed to account for the nondiagonal nature of the model. The

eigenvalues depend on two sets of Bethe roots, for which coupled Bethe ansatz equations have been presented.

An interesting aspect of the model's solution is that, unlike in the case of the XXZ model with nondiagonal boundary conditions, no restrictions emerge for the boundary parameters. This extra freedom, as well as the remnants of particle number conservation leading to sectors of the Hilbert space labelled by the integer M appear to be inherited from the supersymmetric nature of the model. Furthermore, supersymmetry heavily restricts the structure of the eigenvectors and has rendered possible to exactly compute the $M = 0$ eigenstate of the model. A more detailed analysis should provide the complete expressions of all eigenvectors.

Since supersymmetry lifted any possible constraints between the boundary parameters for the small polaron, it is interesting to consider other supersymmetric models with non-diagonal boundaries. Particularly interesting would be an extension of the analysis of the supersymmetric t-J model with open boundaries [29, 30] to this case. In this case nondiagonal terms breaking either the $U(1)$ charge symmetry or the $SU(2)$ spin symmetry of the model can be added. While the latter will likely lead to problems similar to those encountered in the XXZ spin model, we expect that terms breaking the charge symmetry can be dealt with in a similar manner as in the small polaron model.

Another route to follow is to consider operator valued representations of the reflection algebras [7, 31, 32] instead of c -number solutions, and attempt to solve the model for boundary conditions breaking the bulk symmetries. The construction of suitable, generalized Jordan-Wigner transformations for the nondiagonal boundary terms would provide valuable information in this spirit.

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